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Three-Dimensional Simulations of Compressible Turbulence on Leading-Edge Parallel Platforms

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Abstract

A parallelized, three-dimensional hydrodynamics code based on the Piecewise Parabolic Method is used to examine compressible fluid turbulence in three dimensions. We consider both Direct Numerical Simulation and Large Eddy Simulation; in the latter case the idea is to run at coarser resolution through Subgrid-Scale parameterization. Applications include Rayleigh-Taylor and Richtmyer-Meshkov instability and turbulent mixing, and interactions of a shock with pre-existing turbulence. The code has recently been coupled with a radiation diffusion package, which uses an implicit solution technique in three dimensions. Issues of current relevance include parallel efficiency of the 3-D implicit solver, parallel I/O, and post-processing and storage of large data sets. We present performance results on leading-edge platforms, including those supported under the DOE Accelerated Strategic Computing Initiative (ASCI).

Direct Numerical Simulation vs Large Eddy Simulation

- Direct Numerical Simulation (DNS)
  - solve PDEs over all relevant length scales
  - high resolution grid required

- Large Eddy Simulation (LES)
  - represent medium to large scales on the computational grid
  - use closure theory to model effects of small scales
  - not as much gridpoints required as with DNS

Piecewise Parabolic Method (PPM) Code

- Higher-order Godunov method (Colella and Woodward) designed for flows with shocks
- Optional Navier-Stokes terms
- Lagrangian with Eulerian remap
- Directional splitting
- FORTRAN
- 3-D logically rectangular domain decomposition with message-passing
- Communications decomposed into 1-D shifts
- Over 2700 operations per gridpoint per timestep
- 7-Row border (redundant computation to save on communications)

Data Assimilation

- Restart dumps, compressed dumps (2-byte or 1-byte integer)
- Each node produces its own data file
- Data analyzed with PPM tool kit from the University of Minnesota
  - a3d program computes vorticity, power spectra, etc. from individual nodal files
  - a3d can convert to either ascii or bricks-of-bytes (BOB) format
  - Various visualization tools (e.g., PERPATH, BOB) can view BOB format

Comparing Machine Performance

- Common norm of throughput per node/processor must be taken in context
  - processor power
  - processor cost
- ASCI machines are evolving rapidly

Intermachine Comparison

Machine	μs / Δt / point	Mflop / node
LLNL IBM-SP	3.3	25.7
LLNL Cray-T3D	6.4	13.2
Sandia Intel Paragon	21.9	3.9
Sandia Intel ASCI-Red	3.1	27.7
Sandia Intel ASCI-Red	2.4	35.3
Dec Alpha (NE)-1 proc. (Estimate for 32 processors)	23.8 (1.1)	114.0 (78.8)

32-bit
64-bit

Triply periodic decay problem
128-cubed grid
4 x 4 x 2 domain decomposition (32 processors)

Parallel Efficiency on IBM-SP System

No. of nodes	Decomposition	Local mesh	μs / Δt / meshpoint
8	2 x 2 x 2	64 x 64 x 64	10.5
32	4 x 4 x 2	32 x 32 x 64	3.3
128	4 x 4 x 8	32 x 32 x 16	1.2

- Drop in parallel efficiency due almost entirely to redundant border computations

Parallel Efficiency on ASCI-Red System

No. of nodes	Decomposition	Local mesh	μs / Δt / meshpoint
8	2 x 2 x 2	64 x 64 x 64	9.1
32	4 x 4 x 2	32 x 32 x 64	2.4
128	4 x 4 x 8	32 x 32 x 16	0.9

- Drop in parallel efficiency due almost entirely to redundant border computations

Scaling with Increasing Problem Size on Intel Paragon

No. of Nodes	Global mesh	Decomp.	Local mesh	μs / Δt / local-point
8	64 x 64 x 64	2 x 2 x 2	32 x 32 x 32	89.3
512	256 x 256 x 256	8 x 8 x 8	32 x 32 x 32	91.6

- Scaling is almost perfect

Coupling of Radiation Diffusion Package with PPM

- One-group or multigroup flux limited diffusion
- Two-temperature (gas + radiation)
- One equation of state (to be generalized shortly)
- PPM module advects radiation energy-density
- Radiation module addresses effects of radiative absorption and emission
- Radiative acceleration treated as forward-in-time body force
- Spatial differencing of flux divergence leads to 7-point stencil; resulting linear system solved by GMRES with preconditioning, using AZTEC sparse parallel solver

Scaling of AZTEC Solver with Increasing Problem Size on IBM ASCI Blue-Pacific

No. of Nodes	Global mesh	Decomp.	Local mesh	Mflops/ node
1	32 x 32 x 32	1 x 1 x 1	32 x 32 x 32	21.6
8	64 x 64 x 64	2 x 2 x 2	32 x 32 x 32	20.5
64	128 x 128 x 128	4 x 4 x 4	32 x 32 x 32	18.3

High-Resolution Computation on IBM-SP ASCI Blue-Pacific ID System

- 512 x 512 x 512 global mesh
- 128 nodes (4 x 4 x 8 domain decomposition)
- 100 timesteps takes 3 hours
- Restart dump (78 MB / node) takes 7 minutes writing directly to PIOFS file system
- Compressed data dump (13 MB / node) takes 5 minutes

High-Resolution Computation on Intel Tflops ASCI Red System

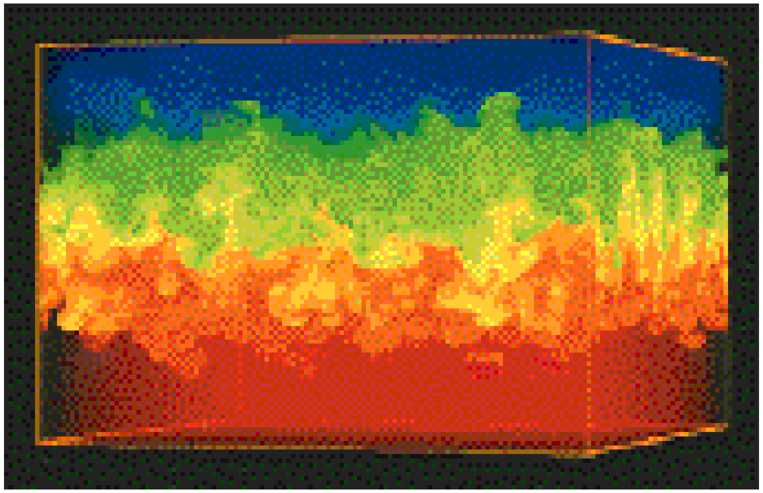
- 512 x 512 x 512 global mesh
- 512 nodes (8 x 8 x 8 domain decomposition)
- 100 timesteps takes 40 minutes
- Restart dump (24 MB / node) takes 12 minutes writing directly to PFS file system
- Compressed data dump (3 MB / node) takes 13 minutes (this involves several hundred separate writes; PFS exhibits very high latency; I/O must be buffered).

Rayleigh-Taylor Instability

- Light fluid trying to support heavy fluid
  - air supporting water
  - astrophysics
  - inertial confinement fusion
- Perturbations at fluid interface grow
- Mixing layer develops
  - heavier fluid forms spikes as it drops into a lighter fluid
  - lighter fluid forms bubbles as it rises into a heavier fluid

Rayleigh-Taylor Simulation on the ASCI Blue Pacific ID System

- Three-dimensional, compressible Navier-Stokes
- Piecewise Parabolic Method (PPM)
- $512 \times 512 \times 512$ resolution
- Ideal gas, $\gamma = 5 / 3$
- Atwood number = 1 / 3
- Prandtl number (ν / κ) = 1
- Viscosity ($\nu / c_s L_z$) = 4×10^{-5}



Richtmyer-Meshkov Instability

- Impulsive-acceleration limit of Rayleigh-Taylor instability
  - shock crosses interface of two fluids of differing density
- Perturbations at fluid interface grow
- Mixing layer with bubbles and spikes develops

Richtmyer-Meshkov Simulation on the ASCI Blue Pacific ID System

- Box size: 0.5 x 0.5 x 1.37
- 192 x 192 x 448 mesh (expanding in *z* at box ends)
- Contact discontinuity with 2-fold density contrast is hit by Mach-6 shock (on low density side)
- Single mode initial perturbation
- Prandtl number = 1.0, viscosity = 4×10^{-5}
- Passive scalar monitors mix

Richtmyer-Meshkov Simulation, cont.

- Second Mach-6 shock launched either from same side or from opposite side
- Smearing of fine-scale structure
- Fluid compresses; mixed layer width then increases significantly
- When shock is from opposite side, there is inversion followed by similar behavior

Toward the Future

- PPM is effective tool for simulating 3-D compressible turbulence
- High resolution (up to billions of zones) will be needed to develop and validate SGS closures
- We will investigate modification of programming model to accommodate distributed-shared-memory (DSM) architectures
- Robust I/O and post processing environment needed for data assimilation
- We will need a lot of computer time (and disk)

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